4-22-2020

Developing Perfectly Matched Layer method to solve Heat Equation numerically

Richard Whitehill
Fort Hays State University, rmwhitehill2@mail.fhsu.edu

Clifton D. Clark
Fort Hays State University, cdclark@fhsu.edu

Developing Perfectly Matched Layer method to solve Heat Equation numerically

FORT HAYS STATE UNIVERSITY
Forward thinking. World ready.

Richard Whitehill, C.D. Clark III
Department of Physics

Abstract

Perfectly Matched Layer (PML) techniques, although having been studied extensively to study systems with nonrestrictive boundaries in many physical fields, are not readily adaptable to the study of thermodynamic systems governed by the heat equation. Using the explicit finite difference method, we can easily describe systems with perfectly absorbing or reflecting boundaries. These, however, are highly idealized physical states, so we have begun extending our abilities to simulating more realistic physical situations by defining arbitrary spatial differential operators, which govern how heat at the boundaries of the system of interest propagates. As a first attempt, we transformed the linear spatial domain to a trigonometric domain to combat reflection from boundaries, but this is quite crude. We then approached the problem using Fourier Transforms in order to define the problem in a heat distribution's frequency space, damp excessive heat past the boundaries, and transform back to position space. Initial results using the finite difference method verify the current computer simulation's ability to solve problems with ideal circumstances, and the development of a PML method which accurately simulates nonrestrictive boundaries and can be easily translated into a computer algorithm is in progress.

Introduction

The theory for numerically solving ordinary and partial differential equations is an expansive one, and its application is broad and well developed, especially as it pertains to the field of computational physics. Generally, we understand how to simulate isolated physical systems with definite boundary conditions with high accuracy, and in many fields – electromagnetism for example – we know how to simulate systems that are open to external influences without much difficulty using the methods of Perfectly Matched Layers (PML). However, when considering the heat equation

$$\rho c \frac{\partial u}{\partial t} = \vec{\nabla} \cdot \kappa \vec{\nabla} u$$

where ρ indicates the material density, c the heat capacity of the material, and κ the conductivity function over the material domain, such PML methods are not incredibly sophisticated or refined, so for this project we are attempting to develop and implement a PML computational model concerning those open systems which places a pseudo-domain layer bordering the real domain over which we are interested such that the data in the real domain is not negatively impacted by the finite nature of our simulations or the imposition of boundary conditions.

Methods

To begin the discussion of the problem, we reduce the heat equation to one equation to reduce the unnecessary complexity and allow the results to be more easily seen on different plots:

$$\rho c \frac{\partial u}{\partial t} = \frac{\partial \kappa}{\partial x}\frac{\partial u}{\partial x} + \kappa \frac{\partial^2 u}{\partial x^2}$$

We implement this equation into a computer simulation using the explicit finite difference method, which is based off of Taylor's theorem shown below.

$$f(x + \Delta x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x)}{n!} \Delta x^n$$

From this theorem, we can derive the first and second order derivatives in the heat equation, neglecting errors from higher order terms in Taylor's expansion). Noting that $u_j^k = u(j\Delta x, k\Delta t)$. With these approximations, the one-dimensional heat equation becomes the following algebraic equation, showing how previous heat distributions evolve over time at each position.

$$u_j^{k+1} = \frac{\Delta t}{4\rho c \Delta x^2}\left(\kappa_{j+1} + 4\kappa_j - \kappa_{j-1}\right)u_{j-1}^k +$$

$$\left(1 - \frac{2\Delta t}{\rho c \Delta x^2}\kappa_j\right)u_j^k + \frac{\Delta t}{4\rho c \Delta x^2}\left(\kappa_{j-1} + 4\kappa_j - \kappa_{j+1}\right)u_{j+1}^k$$

With this expression we can consider two types of boundary conditions.

- 1: hold the values of the heat distribution constant at the extreme values of the linear spatial domain
- 2: we could hold the values of the heat distribution's first derivative at the boundaries constant

By imposing these conditions, we can easily create a step matrix that evolves the heat distribution forward in time. This method outlined is useful when looking at systems with definite boundaries, but it does not work nearly as well when heat is free to flow arbitrarily far away from regions of interest.

As a first attempt at combating this we devised a simple substitution of the form

$$x = L \tan \theta$$

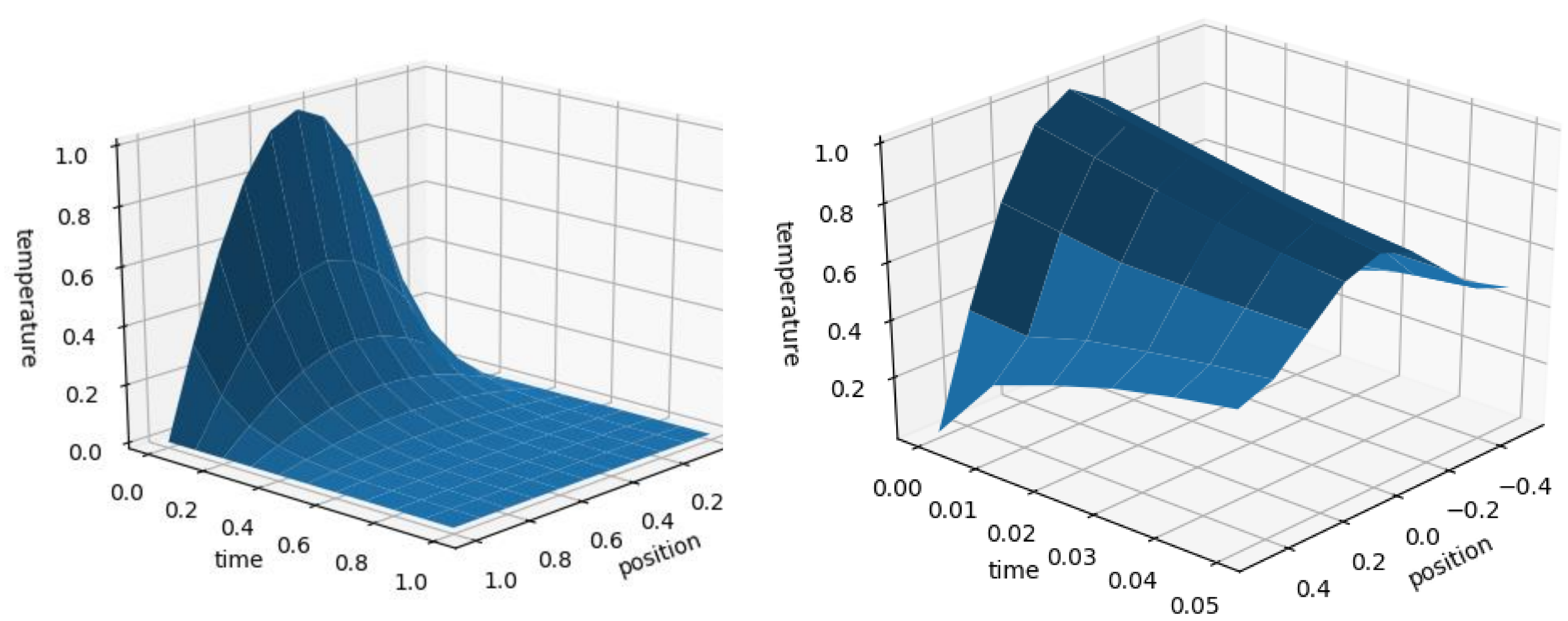
since the tangent function allows us to transform a finite linear spatial domain to an infinite angular one, with varying resolution as dictated by the constant L. In considering this substitution, the heat equation becomes

$$\rho c \frac{\partial u}{\partial t} = \frac{\cos^4 \theta}{L^2}\left[\frac{\partial \kappa}{\partial \theta}\frac{\partial u}{\partial \theta} + \kappa \frac{\partial^2 u}{\partial \theta^2}\right] - \frac{\cos^2 \theta \sin 2\theta}{L^2}\kappa \frac{\partial u}{\partial \theta}$$

which can be turned into an algebraic equation similar to that of the linear spatial case, albeit more complicated, using the finite difference method. From this, we can consider a spatial domain with some excess at the boundaries, apply one of the two boundary conditions which will affect the interesting domain the least from reflection, and write a step matrix again to evolve the system forward in time. After simulating the heat distribution's evolution, we can then transform back to the linear domain to compare solutions obtained by both methods or compare with exact solutions obtained by solving the heat equation for specific cases.

Results

In testing the method implemented without any PMLs, we compared data from computer simulations evolved from an initial temperature distribution for who's future appearance we could analytically predict without ambiguity.



(a) (b)

Figure 1: (a) Temperature evolution of initial heat distribution $u(x,0) = \sin(\pi x)$ with boundary temperatures remaining constant at 0 (b) Temperature evolution of $u(x,0) = \cos(\pi x)$ with boundary temperature's first derivative remaining constant at 0

It can be seen that the sinusoidal functions initially put into the model both exponentially decayed over time. For Fig. 1(a), the heat which reached the boundaries was perfectly taken out of the system, meaning that the system reached an equilibrium at the boundary temperature, and for the system in Fig. 1(b), the heat which reached the boundaries was perfectly reflected back into the region of interest, implying that the system reached a higher temperature at equilibrium. For the $x = L \tan \theta$ substitution, we ran tests similar to those of the non-PML method, only expanding the domain to allow heat at the boundaries to adequately dissipate before greatly impacting the region of interest. Again, the initial temperature distribution put into the simulation which produced Fig. 2 decayed over time, approaching a stable equilibrium.

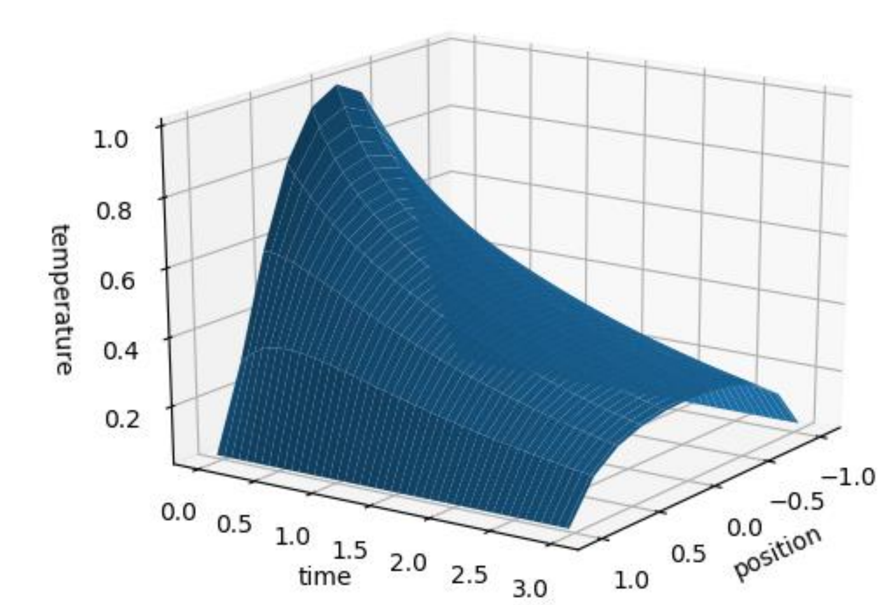


Figure 2: Temperature evolution of a Guassian distribution ($u(x,0) = e^{-x^2}$) which exponentially decays over time with a gradually widening peak

Discussion

Most of the preliminary results presented here are not incredibly consequential with regards to the PML method development or the effectiveness of such a method. Rather, they are mostly validation of computer models tested against analytic solutions. However, we can see in our initial models that our solutions match our expectations well, where the initial temperature function distributes heat among each part of the discretized region of interest, so we know that our models are valid and obey the heat equation when considering isolated systems with definite boundary conditions.

Conclusion

For this project we have thus far implemented a standard computer model for solving the heat equation, which is a partial differential equation dictating how a heat distribution changes over time, and for this model we have utilized the finite difference method to help us write an algebraic relation between the temperature at a point at two different time. Additionally, we have tested a trigonometric substitution which maps a finite linear domain to an arbitrarily large angular domain, and while this method decreases the impact of imposing incorrect boundary conditions on a region, we see that the effects of heat reflection at the boundaries are still quite evident. To combat this we are developing a PML method inspired by Lantos and Nataf (2010) which introduces a new spatial derivative operator for external regions such that the heat which propagates away from the region of interest is exponentially damped. This will hopefully allow us to negate the effects of imposing boundary conditions on a finite domain and accurately simulate how heat in a non-isolated system evolves over time.

References

Lantos, N., & Nataf, F. (2010). Perfectly Matched Layers for the heat and advection-diffusion equations. hal-00454089